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OVERSMART – A Solution Monitoring And Reporting Tool for the OVERFLOW Flow Solver

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A new software tool has been developed to provide a comprehensive report of solution convergence of flow computations over large complex grid systems. The new tool produces a one-page executive summary of the behavior of flow equations residuals, turbulence model equations residuals, and component forces and moments. Under the automatic option, a matrix of commonly-viewed plots such as residual histograms, composite residuals, sub-iteration bar graphs, and component forces and moments is automatically generated. Specific plots required by the user can also be prescribed via a command file or a graphical user interface. Output is directed to the user's computer screen and to an html file for archival purposes. The current implementation has been targeted for the OVERFLOW flow solver but the framework allows easy extension to other flow solvers. The software has been demonstrated to rapidly process large residual history files with millions of lines of data.

I. Introduction

STRUCTURED grid flow solvers such as NASA's OVERFLOW compressible Navier-Stokes flow solver[1,2] can generate large data files that contain convergence histories for flow equations residuals, turbulence model equations residuals, component forces and moments, species convection equations residuals (for multi-species computations), and component relative motion dynamics variables (for prescribed and 6-DOF motion computations). Most existing convergence history analysis tools were designed over a decade ago for a small number of grids and cases (dozens of grids and around 10 million grid points). An example of such a tool is OVERPLOT from the Chimera Grid Tools[3] package (Fig. 1). With the advent in computing technology, most of today's large-scale problems can easily extend to hundreds of grids, and over 100 million grid points.[4–6] However, due to the lack of convenient and efficient tools, only a small fraction of information contained in these files is typically analyzed. A common approach is to construct specific scripts to extract different information from these history files. The disadvantage of these scripts is that they are typically not easily extensible to more general cases and they often lack the capability to quickly examine a high level summary of the convergence histories of all relevant variables.

The goal of the present work is to develop a framework for generating a comprehensive solution convergence report based on the output history files from a flow solver for large-scale configurations. The current implementation is targeted for the OVERFLOW flow solver, but the software can be easily modified to handle other flow solvers. The information returned is designed to be concise and the output is generated quickly with minimal user input, e.g., one screen executive summary of important statistics. Problem areas in convergence are made to be easily identifiable.

The software tool developed to accomplish the above goals is called OVERSMART (stands for OVERFLOW Solution Monitoring And Reporting Tool). In the sections to follow, the software design details are presented. New types of residual statistics graphs are introduced. Execution of the software in command-line and graphical user-interface (GUI) modes are described. Results and timing for several test cases are discussed. Finally, summary and conclusions are provided.

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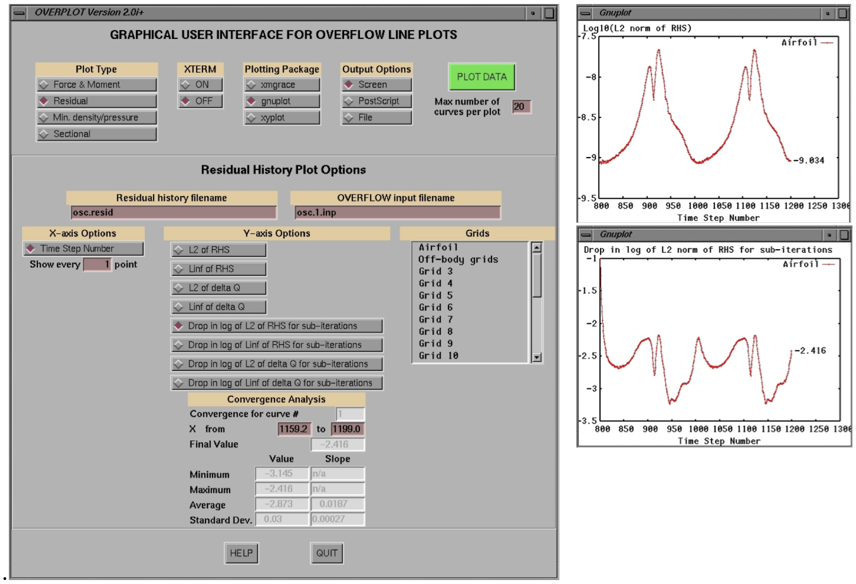


Figure 1. Flow convergence histories analysis with OVERPLOT using one plot, one run at a time paradigm.

II. Software Design

OVERSMART has been designed to generate its output with minimum user input, thus making it very easy to use. Two execution modes are available: command-line and GUI. Under the command-line mode, there is an automatic option and a command file option.

The simplest and most commonly used option is the automatic command-line mode where the software is executed by simply typing `oversmart` at the command prompt with no additional arguments. OVERSMART will determine the types of summary graphs to generate based on the available history files in the current directory. The goal is that the user can obtain a one-screen executive summary of important statistics without any additional user inputs. Problem areas in the convergence can be easily identified.

Alternatively, the user may prefer to generate a specific set of graphs with a particular layout. This is accomplish by using the command file mode where the software is executed via a command file. Either the automatic mode or command file mode can be embedded in a script that executes the flow solver, followed by automatic generation of the convergence summary plots. The third option for running OVERSMART is through its graphical user interface (GUI). In this mode, the user can specify the plot types and their layouts, and view the results in an interactive environment.

The graphs generated by OVERSMART are arranged in a row by column matrix format. This layout is fully configurable by the user command file or from the GUI. The current implementation only produces a one-page summary, which is displayed to the screen and also archived in an html file. For some cases, additional pages may be required to fully understand the convergence. Generation of additional summary pages is in the future plans.

OVERSMART is implemented using the Python and C programming languages. The interface between Python and C is handled by SWIG. Command file parsing and top level controls are performed in Python. A comparison of the time required to read the flow residual history files using Python versus C was performed. It was found that C provides faster read time than Python. Hence, file reading and statistical summary calculations are performed in C.

The matrix of graphs is created using either `matplotlib` or `gnuplot`. `Matplotlib` is a Python plotting package with publication quality graphs, auto-scaled lines and fonts, TeX support, and a large selection of useful options. For this reason, the default plot package that OVERSMART uses is `matplotlib`. The user can easily override this option and specify the more widely available `gnuplot` via a command line option. Presently, OVERSMART runs on the Linux, Unix, and Mac OS-X operating systems.

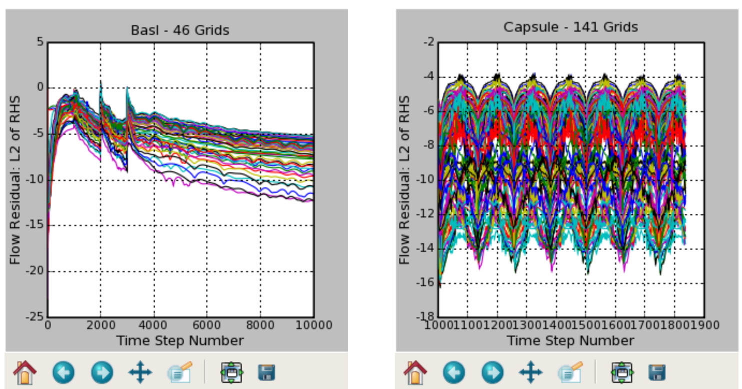
A number of techniques are used to speed-up the data input of the large history files. For simulations with sub-iterations, only the residuals on the first and the last sub-iteration are needed for the order drop statistical summary report. The `fseek` function in C is used to skip reading the "in-between" sub-iterations, resulting in significant savings of the processing time required to generate the graphs. Further large savings in processing time could also be achieved by plotting (and reading) only every N_{skip} time steps for the residual plots, where N_{skip} is a user-controlled optional parameter with a default of 1. Finally, more savings in time is accomplished by storing the history data in-core as far as allowed by the computer's in-core memory.

III. Residual Statistic Graphs

OVERSMART produces three types of residual statistic graphs: histogram, composite, and bar graphs. These are described in more details in the following sub-sections.

III.A. Histogram Summary Statistics

One of the most common measures of solution convergence is the order drop in flow residuals L_2 or L_∞ norm. If there are only a few number of grids, then the analysis can be performed fairly straightforwardly by visually examining the flow residual plot for all grids (Fig. 2a). However, if there are hundreds of grids, it can become quite difficult to determine the order of drops from individual grids (Fig. 2b). A quick and easy way to determine the order of drops for all grids is needed.



(a) (b)

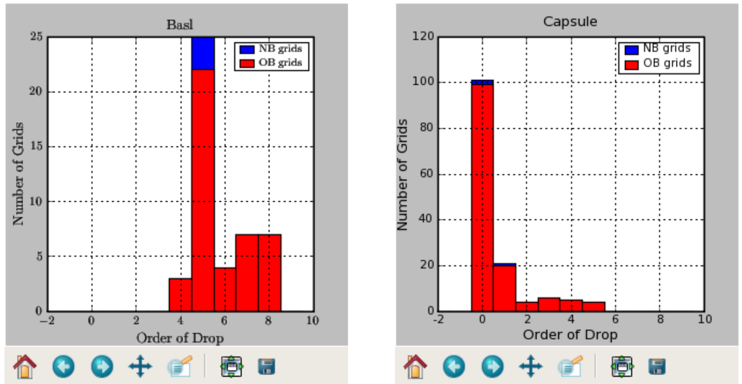
Figure 2. (a) Individual flow residuals from all grids in the 'Basl' data set. The average order drop is around 5.0. (b) Individual residual plots from all grids in the 'Capsule' data set. The order drops from all the grids are nearly impossible to determine.

To address this need, OVERSMART computes the residual order drop histogram. For each grid, it computes the order of drop in flow and turbulence model residuals from the maximum to that of the last time step. Each bin in the histogram represents the magnitude of the order drop. For each bin, the number of grids with the corresponding order drop is determined. OVERSMART also reports the grid numbers of grids belonging to the worst (lowest order drop) and best (highest order drop) bin for convergence. Using this approach, users can easily drill down to investigate those grids with the worst convergence. OVERSMART also provides the option to plot the individual flow residual norms from these two groups of grids.

Figs. 3a and 3b show the histogram plots for the two data sets from Figs 2a and 2b. With the histogram summary statistic, it is now much easier to see the order of drop from the given grids in comparison to Fig. 2. OVERSMART allows users to plot the histogram plots from three groups of grids: near-body, off-body, and all grids. The stacked histograms shown in Fig. 3 are based on two selected groups of grids: near-body grids and off-body grids. Near-body grids are defined to be grids that contain either an inviscid or a viscous wall. Off-body grids are defined to be the remaining grids away from the solid surface of the body, and are typically Cartesian in the overset grid approach.

III.B. Composite Summary Statistics

Another type of flow residual summary statistics is based on the composites of the residual history plots for a selected group of grids, e.g., near-body and off-body. OVERSMART computes a composite residual from



(a) (b)

Figure 3. (a) Histogram plot of the number of grids over order drop in residuals from 46 grids in the 'Basl' data set. Each color bar represents the number of grids with the corresponding order drop. The near-body grids (blue blocks) are stacked on top of the off body grids (red blocks). For the 'Basl' data set, the near-body grids (grids 1, 2, and 3) have an order of drop of 5.0. The grids with the worst order drop of 4.0 are grids 4, 8, and 12 as reported by OVERSMART. (b) Histogram plot of the number of grids over order drop in residuals from 141 grids in the 'Capsule' data set. There are 101 grids with an order drop of 0.0 (due to unsteady motion) and four grids with the best order drop of 5.0: grids 40, 77, 91, and 93 as reported by OVERSMART.

the weighted sum of the flow residuals for each grid. The weights w_i are given by the number of grid points in grid i divided by the total number of points in the grid system. The composite plots give an averaged measure of the behavior of the residual history from each selected group of grids (Fig. 4)

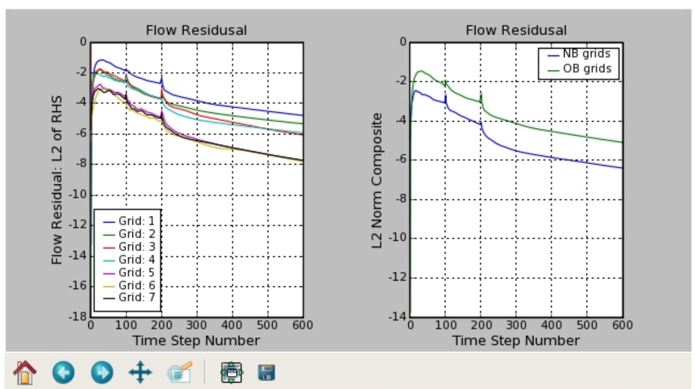


Figure 4. Left graph shows the residual history from seven grids. Right graph shows the composite summary based on the near-body grids (grid 1, 2, and 3) and the off-body grids (grids 4-7).

III.C. Sub-Iteration Order Drop Summary Statistics

For computations with dual time or Newton sub-iterations, it has been difficult to assess the sub-iteration convergence for all grids over all time steps due to the large volume of data that needs to be plotted, e.g., a 100-grid system with 5,000 time steps, and 10 sub-iterations per time step contains 5 million data points.

Since sub-iteration convergence is typically measured by the order drop in residual between the first and the last sub-iteration, it is sufficient to read the residual of just the first and last sub-iteration only. OVERSMART provides an overview of the sub-iteration convergence by showing bar graphs of the minimum, maximum, and average order drop in sub-iteration residuals for each grid over all time steps (Fig. 5). For each grid, a vertical bar is plotted where the lower and upper extremes of the bar mark the minimum and maximum order drop in sub-iteration residuals over all the time steps in the computation. A filled circle between the lower and upper extremes of the bar marks the average order drop in sub-iteration residuals over all time steps. This new summary graph offers the user a quick way to assess how well the sub-iterations are converging without having to plot all the sub-iterations from all time steps for all grids.

Fig. 5 shows the sub-iteration order drop summary graph for the V-22 data set with 51 grids, 11,740 time steps, and 15 sub-iterations per time step. The near-body grids are contained in grids 1 to 12, while multi-level off-body Cartesian grids[7] occupy the remainder of the domain. Level-1 off-body grids are grids 13-16, level-2 off-body grids are grids 17-22, etc. The figure indicates that the near-body grids have a sub-iteration order drop around 2.0, and the level-1 grids have a sub-iteration order drop slightly greater than 4.0. The order drop improves for higher level grids, then decreases for grids 41 to 51.

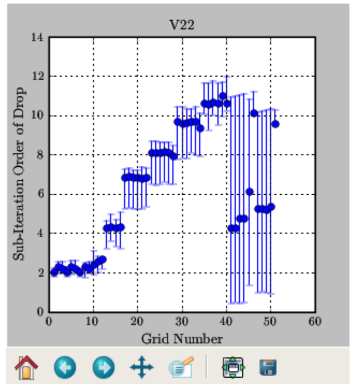


Figure 5. Sub-iteration order drop summary graph for the V-22 data set with 51 grids, 11,740 time steps, and 15 sub-iterations per time step.

IV. Command-Line Execution Mode

In command-line execution mode (or scriptable mode), OVERSMART provides two options: (1) automatic summary page option and (2) user-customized summary page option. Under the command-line mode, execution can be performed at the system command prompt, in background or from a script, and no GUI is invoked. This section describes the two command-line mode options in more detail.

IV.A. Automatic Summary Page

This is the most popular and easy-to-use option because there is no user input required. Users simply type `oversmart` from the system command prompt in the directory containing the run history files and OVERSMART will perform the following steps by default:

1. Search for the following files:
    - Any flow residual, turbulence model residual, force/moment history files in the current directory (for OVERFLOW runs, these files have extensions .resid, .turb, and .fomoco, respectively),
    - Grid file containing grid dimensions information used in computing grid weights for the composite residual plots (for OVERFLOW runs, grid files are names grid.in or x.save), and
    - Flow solver input parameters file (for OVERFLOW runs, this file has extension .inp).
2. Automatically select the most-commonly viewed graphs to generate in the 1-page convergence summary report based on the types of history files found.
3. Compute and plot the selected graphs in the summary page with a default plot matrix template.

Test cases from the OVERFLOW version 2.1s were used for testing purposes. Figs. 6, 7, and 8 show the summary page generated by OVERSMART using the automatic summary page option. Note that for all of these summary pages, it took only a few seconds to generate on a Linux Opteron desktop workstation.

In Fig. 6, the data set consists of 7 grids for a wing-body configuration and no sub-iteration. The first column shows the following summary graphs: the histogram plots of the order of drop over number of grids for the flow residuals L_2 norm (first row), the composite graphs of the flow residuals L_2 norm (second row). The second column shows similar types of summary graphs for the turbulence model equations residuals. It is quickly observed from the turbulence model residuals histogram that there is one grid with a potential convergence problem (with only 1 order drop in residual L_2 norm). The third column shows the X, Y, and Z force coefficients plots and the fourth column shows the X, Y, and Z moment coefficients plots for the wing, body and combined components.

In Fig. 7, the data set consists of 1 grid, no sub-iteration, and no turbulence model. The first column shows the flow residual summary plots as before. Since there is no turbulence model, the second column is blank. The third and fourth columns show the X, Y, and Z force and moment coefficients plots as before.

In Fig. 8, the data set consists of 1 grid and 6 sub-iteration per time step. The first column shows the flow residual histogram and composite plots as before. Now there is a third row plot that shows the sub-iteration order drop summary graph. Since there is only one grid, there is only one bar showing the minimum order drop, the average order drop (denoted by the circle), and the maximum order drop. The second column is blank because there is no turbulence model. The third and fourth columns show the X, Y, and Z force and moment coefficients plots as before. Since this is an oscillating case, the X, Y, and Z force and moment coefficient plots depict the oscillations.

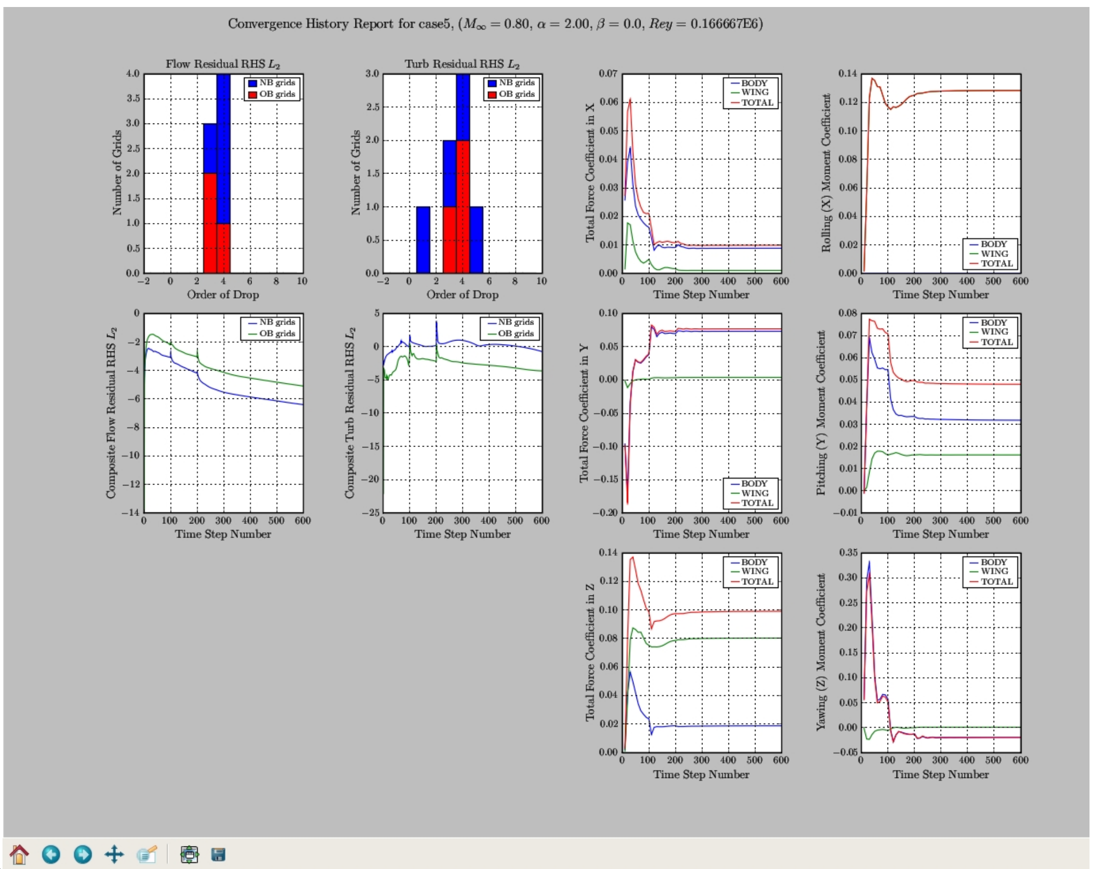


Figure 6. Automatic summary page for the Wing-Body test case.

IV.B. User-Customized Summary Page

Though OVERSMART will automatically detect which summary graphs to generate based on the available history files in the current directory, users may still wish to configure their own summary page at times. This is particularly useful when after studying the automatic summary page, the user wishes to drill down to investigate individual graphs/grids in more details. An optional command file can be used to create the user-customized summary page (invoked by simply typing `oversmart -command cmdfile` at the system command prompt where `cmdfile` is the name of the command file). The command file contains information about the graphs that OVERSMART needs to generate and their row and column positions on the page. For example, the following command file will generate a graph of the Histogram Summary Statistics of the

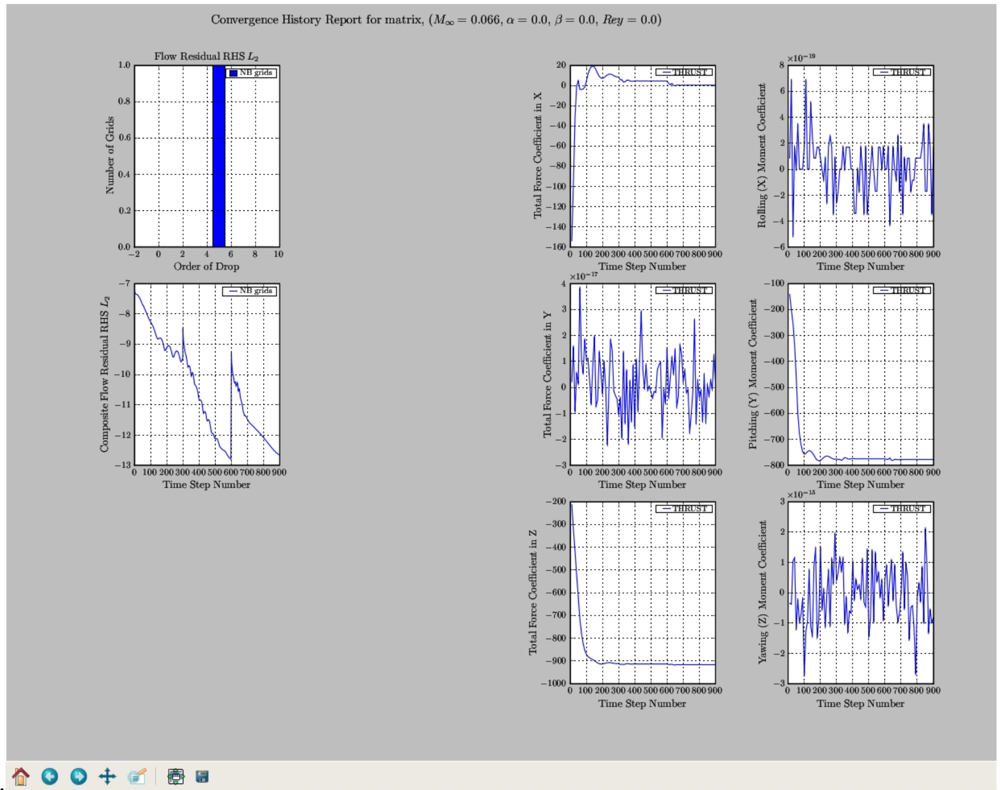


Figure 7. Automatic summary page for the Nozzle test case.

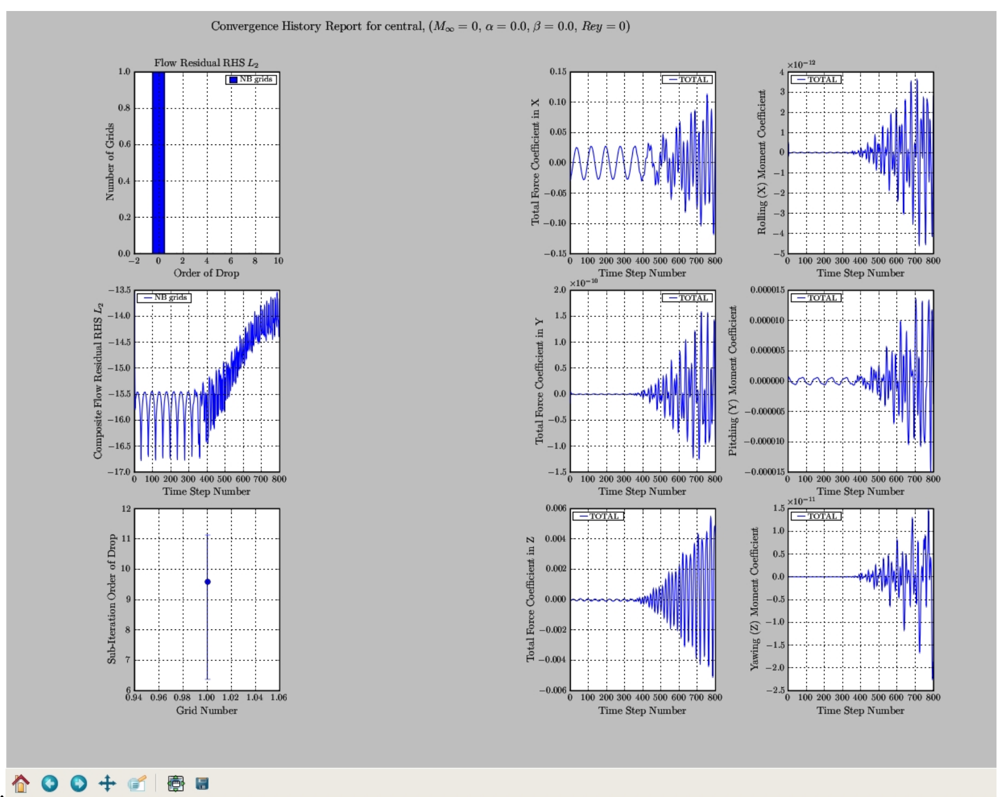


Figure 8. Automatic summary page for the Oscillating Sphere test case.

flow residual L_2 norm for two selected groups of grids: near-body and off-body grids, and position the plot in row 1 and column 1 of the plot matrix.

Resid `SL2`
Grid `Near, Off`
Histogram
Plot `Row 1 Column 1`

The first word at the beginning of each line in the command file is a command and the remaining texts (if any) are the command arguments. The following OVERSMART commands will generate a graph of the Composite Summary Statistics of the L_2 norm flow residual in the command file.

Resid `SL2`
Grid `Near, Off`
Composite
Plot `Row 1 Column 1`

For data with turbulence model, simply change the command `Resid` to `Turb`.

Turb `SL2`
Grid `Near, Off`
Composite
Plot `Row 1 Column 1`

IV.C. HTML Report File

Under command-line execution mode, OVERSMART sends the plot matrix output of the summary page to the computer screen as well as to an html report file. In addition to the summary page plots like the ones shown in Fig. 6, a tabulated summary of the flow and turbulence model residual L_2 norm histograms (Tables 1 and 2), and the final values of the force and moment coefficients for all components (Table 3) are listed in the report file. For the residual tables, all near-body grids are classified by their order drop in residual L_2 norm, while only grids belonging to the worst order drop in residual L_2 norm for off-body grids are tabulated. This html report serves as a valuable and automatically-generated archive for an overview of the convergence characteristics of a run.

Table 1. Flow Residual L_2 Norm Histogram for V-22 case (Figure 13, row 1 column 1)

Grid	Order of Drop	# of Grids	Grid List
Near Body	1.0	6	1, 3, 4, 6, 7, 9
Near Body	2.0	6	2, 5, 8, 10, 11, 12
Off-Body	0.0	12	35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 51

V. GUI Execution Mode

OVERSMART provides a graphical user interface (GUI) to allow users to modify the plot parameters and view the plots interactively. This is particularly useful for beginner users who wish to examine plots that are not generated under the automatic command-line mode. When the command option "`-gui`" is specified, OVERSMART will display the main GUI panel (Fig. 9) instead of running in command-line mode. The main GUI panel allows users to easily browse and select the data sets to be analyzed. The Commands panel (Fig. 10) gives a visual display of the matrix of plots that OVERSMART will generate for the executive summary page. For each sub-plot in the summary page, users can easily change the type of graph and the associate data variable to plot. The user can also save and retrieve previously saved summary page templates. Under the Preferences panel (Fig. 11), plot attributes can be set, saved and retrieved. Configurable plot attributes include the time step skipping parameter N_{skip}, the maximum number of components allowed in

Table 2. **Turbulence Model Residual L_2 Norm Histogram for V-22 case (Figure 13, row 1 column 2)**

Grid	Order of Drop	# of Grids	Grid List
Near Body	1.0	1	6
Near Body	2.0	5	1, 3, 4, 7, 9
Near Body	3.0	1	5
Near Body	4.0	2	2, 8
Near Body	5.0	1	12
Near Body	7.0	1	11
Near Body	9.0	1	10
Off-Body	0.0	20	22, 28, 34, 35, 36, 37, 38, 39, 40, 41 42, 43, 44, 45, 46, 47, 48, 49, 50, 51

Table 3. **Final Force and Moment Coefficient Values for V-22 case. $FX_{tot}, FY_{tot}, FZ_{tot}$ are the total force coefficients in the X, Y, and Z directions respectively; $MX_{tot}, MY_{tot}, MZ_{tot}$ are the total moment coefficients in the X, Y, and Z directions respectively.**

Component	FX_{tot}	FY_{tot}	FZ_{tot}	MX_{tot}	MY_{tot}	MZ_{tot}
CENTERBODY	-9.6011e-07	1.3628e-06	1.6063e-06	9.2183e-08	1.1418e-07	-1.5353e-07
ROTOR	1.2024e-07	-1.0079e-07	0.015153	-7.962e-06	1.1963e-05	-0.0016884

a single force/moment coefficient plot, etc. While experienced users will typically utilize the command-line mode, the GUI mode is still useful and convenient for generating a new template for the plot matrix in the summary page.

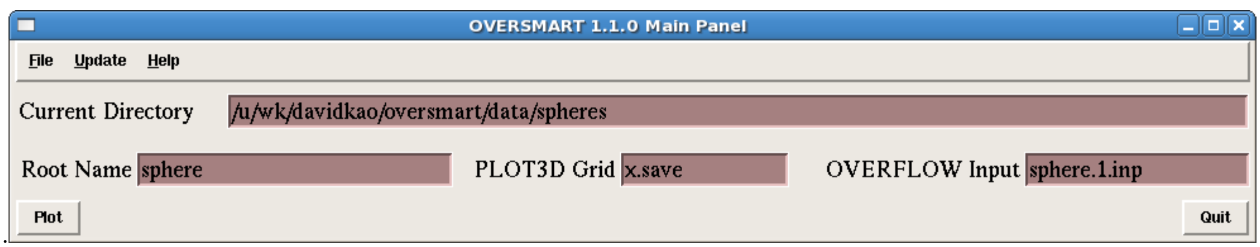


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Figure 9. The Main GUI Panel allows users to easily browse and select the convergence history data files to report. Flow and turbulence model equations residual history files, and component forces and moments history files are automatically selected based on the 'Root Name'.

VI. Results

This section presents results from several large-scale simulations. For each test case, the OVERSMART automatic summary page option was used. The first data set is an oscillating airfoil with turbulence model. The flow residual and the turbulence-model residual history files each contains 880,000 lines. There are 22 grids, 400 time steps and 100 sub-iterations per time step. Without using the `fseek` C function, it took 27 seconds to generate the graphs of the summary page shown in Fig. 12. Using `fseek` to skip read the "in-between" sub-iterations, it takes approximately 1 second to generate these graphs (Table 4).

The second data set is an unsteady flow simulation of the V-22 in hover with turbulence modeling. There are approximately 8 million lines in each of the flow residual and turbulence model residual history files. A total of 11,740 time steps were used for this test case, and each time step has 15 sub-iterations. The V-22 geometry consists of 51 grids, of which 12 grids are the near-body grids and 39 are off-body grids. Table 5 shows the timing result for creating the graphs shown in Fig. 13. Note the 5.8 times speed up with `fseek`. By storing data in-core, it takes only 12 seconds (Table 5) to generate the graphs for the summary page, which is an impressive speed up of a factor of 24 times.

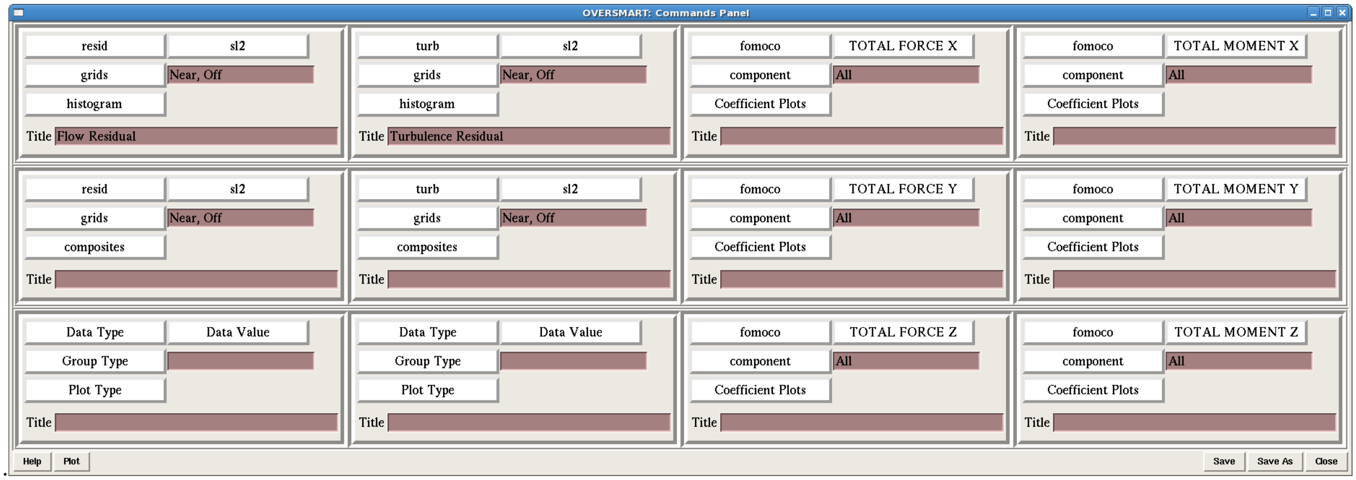

Figure 10. The Commands Panel allows users to easily configure the matrix of plots in the executive summary page that OVERSMART generates.

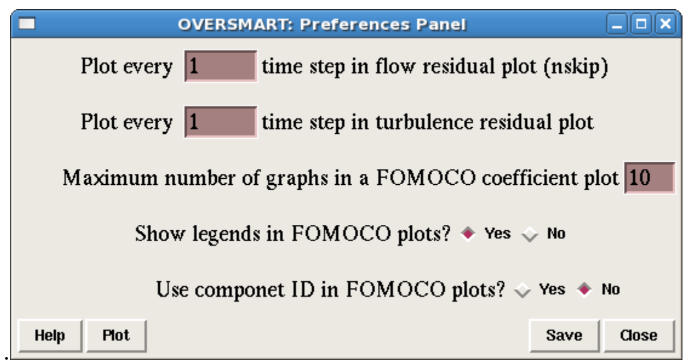

Figure 11. The Preferences Panel allows users to change attributes of the plots.

Table 4. Timing results for the oscillating airfoil automatic summary page. Ran on an Opteron system, 1.0 GHz processor with 1,024 KB cache size.

Airfoil	Total Time	Speed-up
Without fseek	27 s	
With fseek	1 s	27 X

Table 5. Timing results for the V-22 automatic summary page

V-22	Total Time	Speed-up
Without fseek	298 s (4 min 58 s)	
With fseek	51 s	5.8 X
In-Core	12 s	24 X

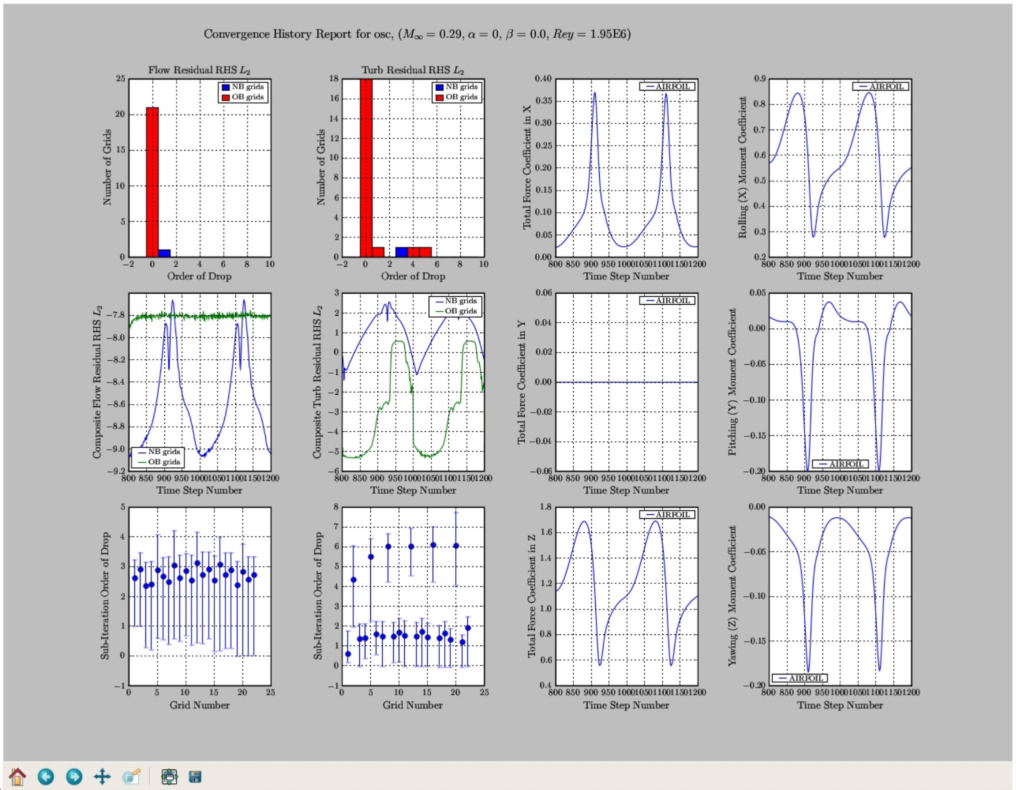

Figure 12. Automatic summary page for the Oscillating Airfoil test case.

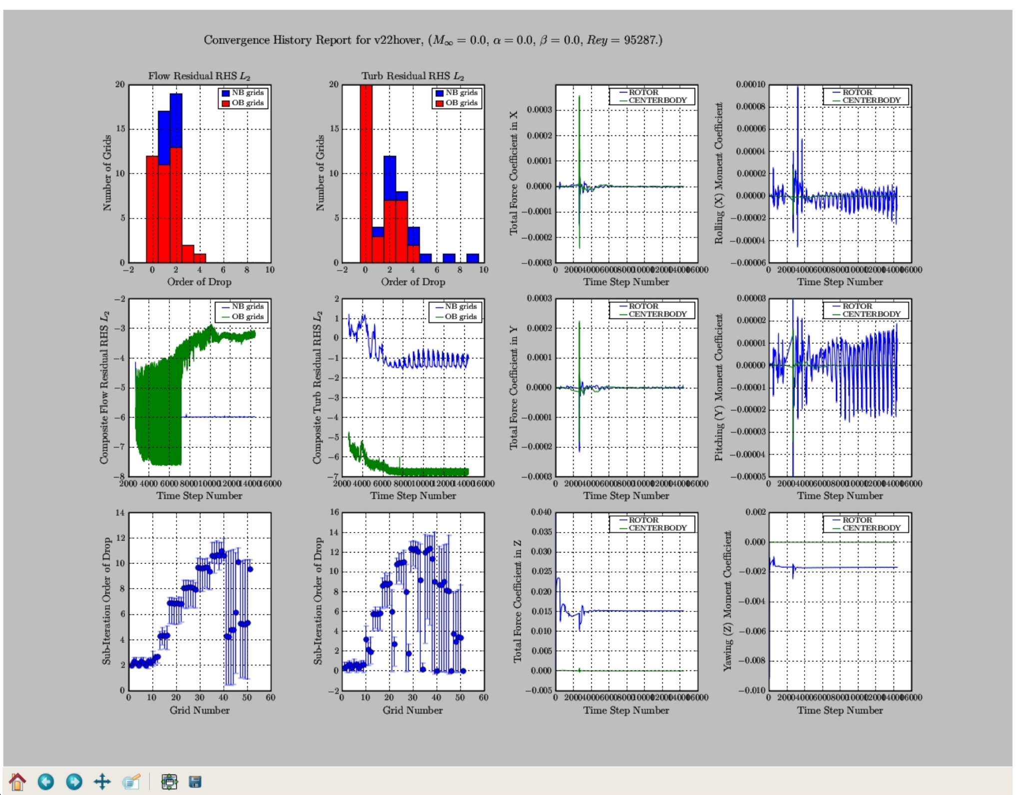

Figure 13. Automatic summary page for the V-22 data set.

The third data set is an unsteady flow simulation of a capsule with turbulence modeling.[8] There are approximately 2.4 million lines in each of the flow residual and turbulence model residual history files. A total of 837 time steps were used for this test case, and each time step has 19 sub-iterations. The capsule geometry consists of 141 grids. Observe from Fig. 14 that approximately 100 grids have zero order drop (due to the unsteady behavior) and only a handful with an order drop of 5.0, which is the best order drop. The sub-iteration order drop graphs also indicate that there is a very low order drop (around 0) for the first 100 or so grids. The grids with the higher order drops are the last few grids (grids 130 and above). Table 6 shows the timing result for creating the graphs shown in Fig. 14. Note the speed up factor of 4.8 by storing data in-core.

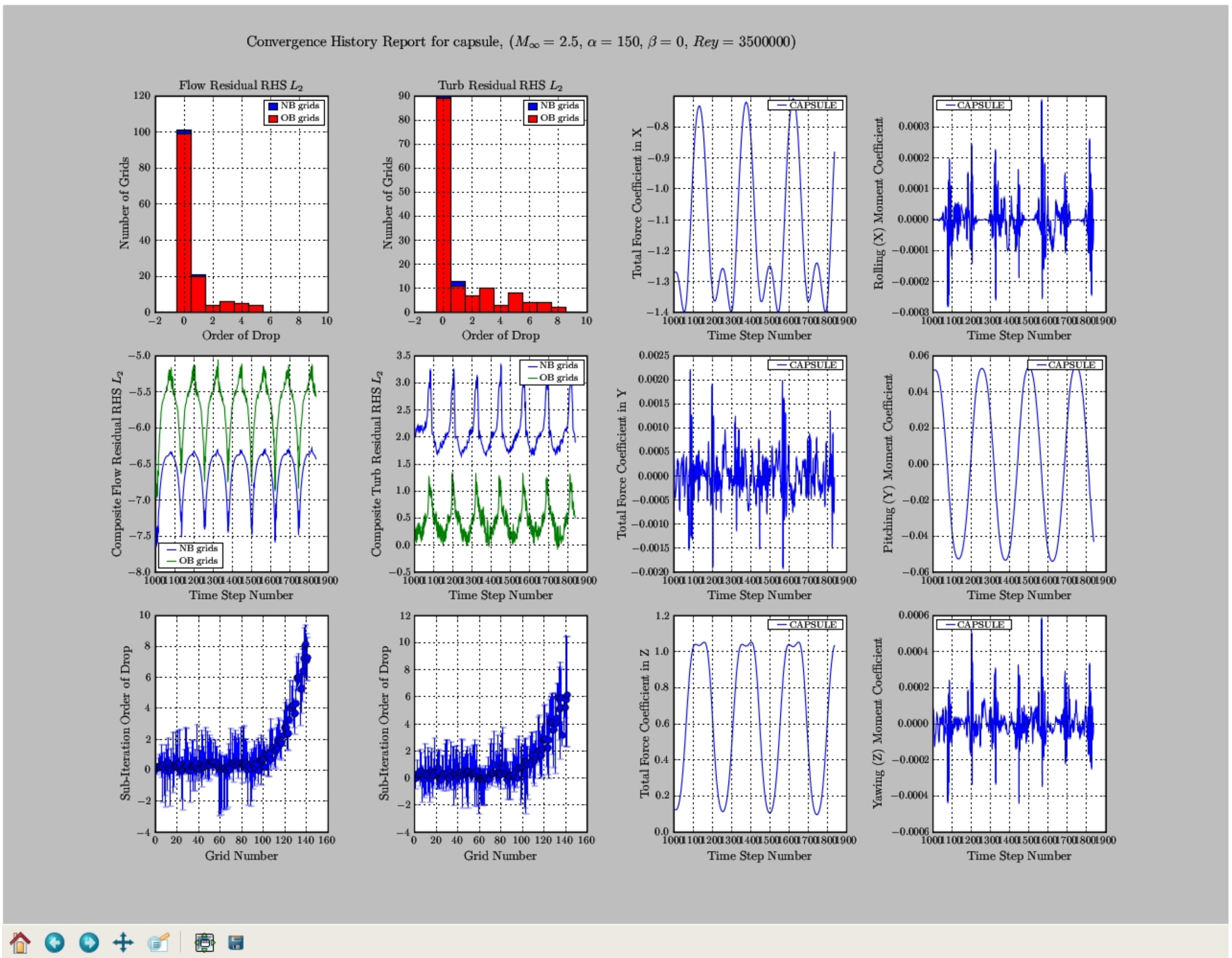

Figure 14. Automatic summary page for the Capsule data set.

Table 6. Timing results for the capsule data with the automatic summary page

Capsule	Total Time	Speed-up
Out-of-core	14 s	
In-core	3.6 s	4.8 X

The last data set is an unsteady flow simulation of the Space Shuttle Launch Vehicle (SSLV) with turbulence modeling.[4] There are approximately 19 million lines of data in each of the flow and turbulence model residual history files. A total of 10,000 time steps were used for this test case, and each time step has 3 sub-iterations. The shuttle geometry consists of 636 grids. Table 7 shows the timing result for creating the graphs shown in Fig. 15. Note the speed up factor of 4.8 by storing data in-core. With this large-scale data, it is very difficult to analyze the convergence history with the current tools. OVERSMART provides a quick way to look for any potential problems in the simulation using the graphs shown in the summary page.

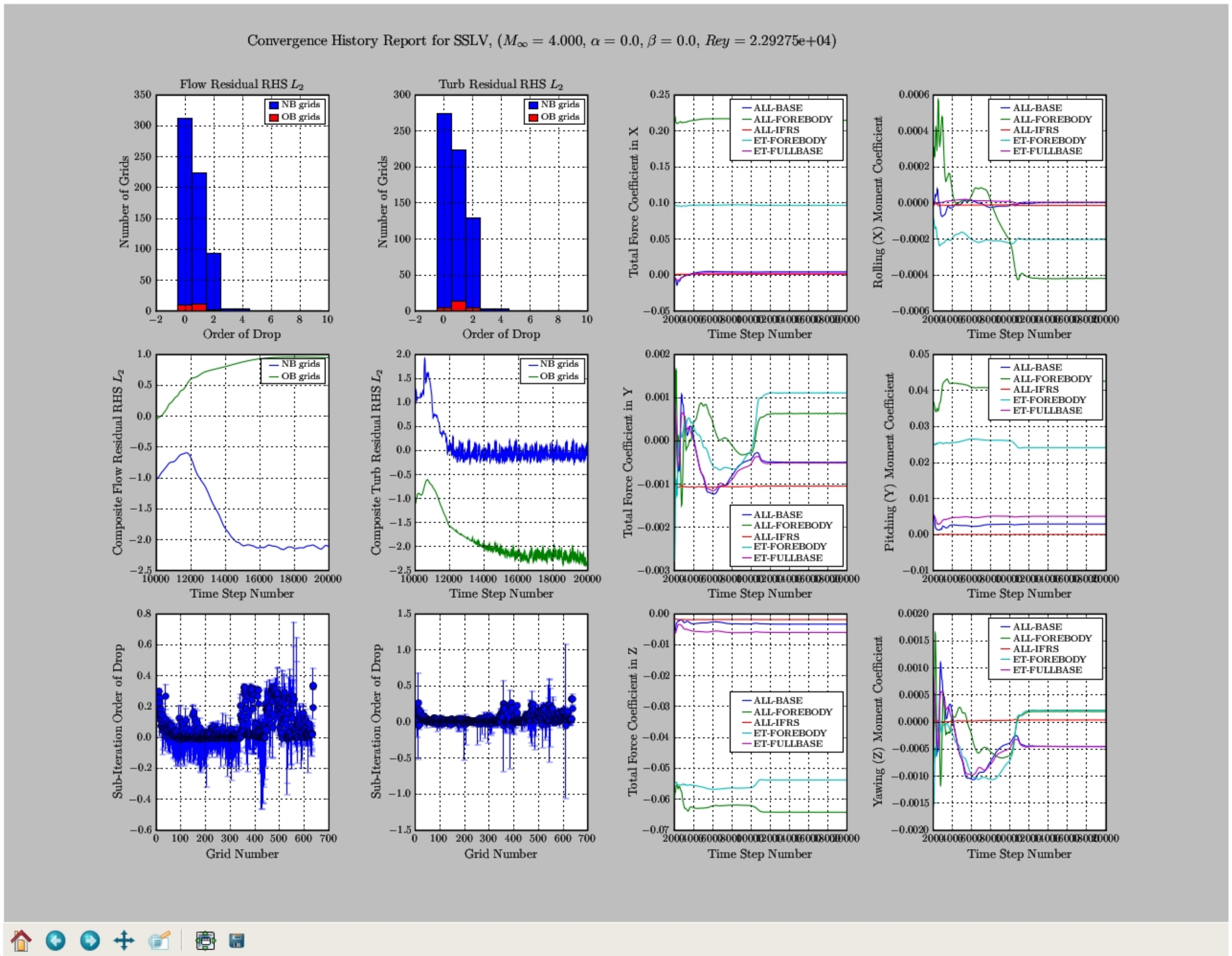

Figure 15. Automatic summary page for the SSLV data set.

Table 7. Timing results for the SSLV data with the automatic summary page

SSLV	Total Time	Speed-up
Out-of-core	28 min 37 s	
In-core	5 min 58 s	4.8 X

VII. Summary, Conclusions and Future Work

With large-scale simulations containing hundreds of grids and millions of lines of history output becoming more common, it is often inconvenient or nearly impossible to perform convergence analysis using current tools. Lack of convergence in a small but maybe significant region of the flow field can easily be missed by the user. OVERSMART is the next-generation tool for easy-to-use and more comprehensive rapid analysis of the convergence behavior of large-scale computations. The executive summary page with the different statistic graphs provides an effective means for users to obtain a quick global view of the convergence histories of important variables in the computation. Problem areas (grids) in convergence can be easily and rapidly identified.

Further work planned beyond the scope of the current paper includes an option to generate multi-page summaries of various convergence plots, a dynamic monitoring mode to view the convergence histories as the flow solver is running, a parallel processing option to make better use of the multiple processors that are now common in most desktop machines, and options to compare convergence plots from several different runs.

VIII. Acknowledgements

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